

# Study of off-diagonal disorder using the typical medium dynamical cluster approximation

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(Dated: June 6, 2014)

We generalize the typical medium dynamical cluster approximation (TMDCA) and the local Blackman, Esterling, and Berk (BEB) method for systems with off-diagonal disorder. Using our extended formalism we perform a systematic study of the effects of non-local disorder-induced correlations and of off-diagonal disorder on the density of states and the mobility edge of the Anderson localized states. We apply our method to the three-dimensional Anderson model with configuration dependent hopping and find fast convergence with modest cluster sizes. Our results are in good agreement with the data obtained using exact diagonalization, and the transfer matrix and kernel polynomial methods.

PACS numbers: 71.27.+a, 02.70.-c, 71.10.Fd, 71.23.An

## I. INTRODUCTION

Disorder which is inevitably present in most materials can dramatically affect their properties.<sup>1,2</sup> It can lead to changes in their electronic structure and transport. One of the most interesting effects of disorder is the spatial confinement of charge carriers due to coherent backscattering off random impurities which is known as Anderson localization.<sup>3,4</sup> Despite progress over the last decades, the subject of Anderson localization remains an active area of research. The lack of quantitative analytical results has meant that numerical investigations (see for e.g., Refs. 5–11) have provided a significant role in understanding the Anderson transition.<sup>12–14</sup>

The simplest model used to study the effects of disorder in materials is a single band tight binding model with a random on-site disorder potential.<sup>15</sup> Such a model is justified when the disorder is introduced by substitutional impurities, as in a binary alloy. The substitution of host atoms by impurities only leads to changes of the local potential on the substitutional site and, on average, does not affect the neighbors.<sup>15,16</sup> In this situation, the disorder appears only in the diagonal terms of the Hamiltonian and hence is referred to as diagonal disorder. However, when the bandwidth of the dopant is very different from the one of the pure host, such substitution results not only in the change of the local potential but may also affect the neighboring sites.<sup>15</sup> Consequently, a simple model to capture such effects should include both random local potentials and random hopping amplitudes which depend on the occupancy of the sites. The dependence of the hopping amplitude on the disorder configuration is usually referred to as off-diagonal disorder. Of course, a proper theoretical description of realistic disordered materials requires the inclusion of both diagonal and off-diagonal randomness.

The coherent potential approximation (CPA) is a widely used single site mean field theory for systems with strictly diagonal disorder.<sup>16</sup> Blackman, Esterling

and Berk (BEB)<sup>17</sup> have extended the CPA to systems with off-diagonal disorder. However, being single-site approximations, the CPA and the BEB theories neglect all disorder induced non-local correlations.

There have been a number of attempts to develop systematic nonlocal extensions to the CPA. These include cluster extensions such as the molecular coherent potential approximation (MCPA),<sup>18,19</sup> the dynamical cluster approximation (DCA),<sup>20–22</sup> etc. Self-consistent mean field studies of off-diagonal disorder have been conducted by a number of authors.<sup>19,23–25</sup> However, all these studies have been performed at the local single-site BEB level. To include the effects of off-diagonal disorder, Gonis<sup>18</sup> extended the Molecular CPA, which uses a self-consistently embedded finite size cluster to capture non-local corrections to the CPA. However, he criticized the MCPA for violating translational invariance and other critical properties of a valid quantum cluster theory.<sup>15,26</sup> In order to take into account such non-local effects on off-diagonal disorder models while maintaining translational invariance, we extend the BEB formalism using the DCA scheme.<sup>20–22</sup>

While the CPA, DCA, and BEB have shown to be successful self-consistent mean-field theories for the quantitative description of the density of states and electronic structure of disordered systems, they can not properly address the physics of Anderson localization. These mean field approaches describe the effective medium using the average density of states which is not critical at the transition.<sup>12,26–28</sup> Thus, theories which rely on such averaged quantities will fail to properly characterize Anderson localization. As noted by Anderson, the probability distribution of the local density of states must be considered, focusing on the most probable or the *typical* value.<sup>3,29</sup> Close to the Anderson transition, the distribution is found to have very long tails characteristic of a log-normal distribution.<sup>10,30,31</sup> In fact, the distribution is log-normal up to ten orders of magnitude<sup>32</sup> and so the typical value<sup>31,33–35</sup> is the geometrical mean. Based on this idea, Dobrosavljević *et al.*<sup>36</sup> formulated a single site

typical medium theory (TMT) for the Anderson localization. This approximation gives a qualitative description of the Anderson localization in three dimensions. However, it fails to properly describe the trajectory of the mobility edge (which separates the extended and localized states) as it neglects non-local corrections and so does not include the effects of coherent backscattering.<sup>37</sup> It also underestimates considerably the critical strength of the disorder at which the localization happens. In addition, TMT is only formulated for diagonal disorder.

Recently, by employing the DCA within the typical medium analysis, we developed a systematic Typical Medium Dynamical Cluster Approximation (TMDCA) formalism.<sup>26</sup> The TMDCA provides an accurate description of the Anderson localization transition for modest cluster sizes in three-dimensional models with diagonal disorder while recovering the TMT for a one-site cluster. In this work, we generalize our recently proposed TMDCA scheme to address the question of electron localization in systems with both diagonal and off-diagonal disorder.

To go beyond the local single-site CPA-like level of the BEB formalism, we employ the DCA<sup>20–22</sup> scheme which systematically incorporates non-local spatial correlations effects. Hence, in this paper, we first present an extension of the DCA for systems with both diagonal and off-diagonal disorder. Next, we develop a typical medium dynamical cluster approximation formalism capable of incorporating the effects of Anderson localization both for diagonal and off-diagonal disorder. We then perform a systematic study of the effects of non-local correlations and off-diagonal randomness on the density of states and electron localization. The results of our calculations are compared with the ones obtained with other numerical methods for finite size lattices, including exact diagonalization, kernel polynomial, and transfer matrix methods.

The paper is organized as follows: following the Introduction in Sec. I we present the model and describe the details of the formalism we used in Sec. II. In Sec. III A we present our results of the average density of states for both diagonal and off-diagonal disorder cases. In Sec. III B we consider the effects of diagonal and off-diagonal disorder on the typical density of states, from which we extract the mobility edges and construct a complete phase diagram in the disorder-energy parameter space. We summarize and discuss future directions in Sec. IV.

## II. FORMALISM

### A. Dynamical cluster approximation for off-diagonal disorder

The simplest model widely used to study disordered systems is the single band tight binding Hamiltonian

$$H = - \sum_{\langle i,j \rangle} t_{ij} (c_i^\dagger c_j + h.c.) + \sum_i v_i n_i, \quad (1)$$

where disorder is modeled by a local potential  $v_i$  which is a random variable with probability distribution function  $P(v_i)$ . We will focus on the binary disorder case, where some host  $A$  atoms are substituted with  $B$  impurities with a probability distribution function of the form

$$P(v_i) = c_A \delta(v_i - V_A) + c_B \delta(v_i - V_B), \quad (2)$$

where  $c_B = 1 - c_A$ . For the diagonal disorder case when the bandwidth of the pure host  $A$  is about the same that the bandwidth of the  $B$  system, such substitution results only in a change of the local potential  $v_i$  at the replaced site  $i$ . This corresponds to changes in the diagonal elements of the Hamiltonian. In this case it is assumed that substitution of impurity atoms on average has no effect on hopping amplitudes to the neighboring atoms.

For systems with off-diagonal disorder, the randomness is introduced not only locally in the random diagonal potential  $v_i$ , but also through the hopping amplitudes. To model this, BEB<sup>17</sup> introduced the disorder configuration dependent hopping amplitude of electrons  $t_{ij}$  as

$$t_{ij} = \begin{cases} t_{ij}^{AA}, & \text{if } i \in A, \quad j \in A \\ t_{ij}^{BB}, & \text{if } i \in B, \quad j \in B \\ t_{ij}^{AB}, & \text{if } i \in A, \quad j \in B \\ t_{ij}^{BA}, & \text{if } i \in B, \quad j \in A, \end{cases} \quad (3)$$

where  $t_{ij}$  depends on the type of ion occupying sites  $i$  and  $j$ . For off-diagonal disorder BEB<sup>17</sup> showed the scalar CPA equation becomes a  $2 \times 2$  matrix equation, with corresponding AA, AB, BA, and BB matrix elements. In momentum space, if there is only near-neighbor hopping between all ions, the bare dispersion can be written as (the under-bar denotes matrices)

$$\underline{\varepsilon}_k = \begin{pmatrix} t^{AA} & t^{AB} \\ t^{BA} & t^{BB} \end{pmatrix} \varepsilon_k \quad (4)$$

where in three dimensions  $\varepsilon_k = -2t(\cos(k_x) + \cos(k_y) + \cos(k_z))$  with  $4t = 1$  which sets our unit of energy, and  $t^{AA}$ ,  $t^{BB}$ ,  $t^{AB}$ , and  $t^{BA}$  are unitless prefactors.

The BEB approach is local by construction, hence all non-local disorder induced correlations are neglected.<sup>17</sup> In order to take into account non-local physics, we extend the BEB formalism to a finite cluster using the DCA scheme. Here in the following, we present the algorithm and details of our non-local DCA extension of the BEB formalism for off-diagonal disorder. Just as in the DCA scheme,<sup>22</sup> the first Brillouin zone is divided into coarse-grained cells with centers  $K$  surrounded by points  $\tilde{k}$  within the cell so that an arbitrary  $k = K + \tilde{k}$ .

For a given DCA  $K$ -dependent effective medium hybridization  $\underline{\Delta}(K, \omega)$  matrix

$$\underline{\Delta}(K, \omega) = \begin{pmatrix} \Delta^{AA}(K, \omega) & \Delta^{AB}(K, \omega) \\ \Delta^{BA}(K, \omega) & \Delta^{BB}(K, \omega) \end{pmatrix} \quad (5)$$

we solve the cluster problem, usually in real space. A set of stochastically generated random configuration of disorder potentials  $v_i$  is used to calculate the disorder averaged cluster Green function  $\overline{G}_c(K, \omega)$ ,

$$(\underline{G}_c)_{ij} = \langle (\underline{\omega} - \underline{\overline{t}}' - \underline{\Delta}' - \underline{\mathbf{V}})_{ij}^{-1} \rangle \quad (6)$$

where  $\langle \dots \rangle$  denotes disorder averaging and  $\underline{\mathbf{V}}$  is a diagonal matrix for the disorder site potential. The primes stand for the configuration dependent Fourier transform (FT) components of the hybridization and hopping, respectively. I.e.,

$$\underline{\Delta}'_{ij} = \begin{cases} FT(\Delta(K, \omega)^{AA}), & \text{if } i \in A, j \in A \\ FT(\Delta(K, \omega)^{BB}), & \text{if } i \in B, j \in B \\ FT(\Delta(K, \omega)^{AB}), & \text{if } i \in A, j \in B \\ FT(\Delta(K, \omega)^{BA}), & \text{if } i \in B, j \in A \end{cases} \quad (7a)$$

and

$$\underline{\overline{t}}'_{ij} = \begin{cases} FT(\overline{t}(K)^{AA}), & \text{if } i \in A, j \in A \\ FT(\overline{t}(K)^{BB}), & \text{if } i \in B, j \in B \\ FT(\overline{t}(K)^{AB}), & \text{if } i \in A, j \in B \\ FT(\overline{t}(K)^{BA}), & \text{if } i \in B, j \in A \end{cases} \quad (7b)$$

with

$$\underline{\overline{t}}(K) = \begin{pmatrix} t^{AA} & t^{AB} \\ t^{BA} & t^{BB} \end{pmatrix} \frac{N_c}{N} \sum_{\vec{k}} \varepsilon_{\vec{k}}, \quad (7c)$$

where  $\underline{\Delta}'_{ij}$  and  $\underline{\overline{t}}'_{ij}$  are  $N_c \times N_c$  real-space matrices (where  $N_c$  is the cluster size), and e.g.,  $FT(\Delta(K, \omega)^{AA}) = \sum_K \Delta(K, \omega)^{AA} e^{iK(r_i - r_j)}$ . The hopping can be long ranged, but since they are coarse-grained quantities are effectively limited to the cluster. Physically,  $\underline{\Delta}'_{ij}$  represents the hybridization between sites  $i$  and  $j$  which is configuration dependent. For example, the AA component of the hybridization corresponds to both A species occupying site  $i$  and  $j$ , while the AB component means that site  $i$  is occupied by an A atom and site  $j$  by a B atom. The interpretation of the hopping matrix is the same as for the hybridization function.

In the next step, we form the  $2N_c \times 2N_c$  disorder averaged Green function

$$\langle G_c(\omega)_{ij} \rangle = \begin{pmatrix} \langle G_c^{AA}(\omega) \rangle_{ij} & \langle G_c^{AB}(\omega) \rangle_{ij} \\ \langle G_c^{BA}(\omega) \rangle_{ij} & \langle G_c^{BB}(\omega) \rangle_{ij} \end{pmatrix}. \quad (8)$$

This may be done by assigning the components according to the occupancy of the sites  $i$  and  $j$

$$\begin{aligned} (G_c^{AA})_{ij} &= (G_c)_{ij} \text{ if } i \in A, j \in A \\ (G_c^{BB})_{ij} &= (G_c)_{ij} \text{ if } i \in B, j \in B \\ (G_c^{AB})_{ij} &= (G_c)_{ij} \text{ if } i \in A, j \in B \\ (G_c^{BA})_{ij} &= (G_c)_{ij} \text{ if } i \in B, j \in A \end{aligned} \quad (9)$$

with the other components being zero. Because only one of the four matrix elements is finite for each disorder configuration (each site can be occupied by either A or B atom), only the sum of the elements in Eq. 8 is normalized as a conventional Green function.

Having formed the configuration dependent average Green function, we then Fourier transform to  $K$ -space (which also imposes translational symmetry) and obtain the  $K$ -dependent disorder averaged cluster Green function for each component of the matrix

$$G_c(K, \omega) = \begin{pmatrix} G_c^{AA}(K, \omega) & G_c^{AB}(K, \omega) \\ G_c^{BA}(K, \omega) & G_c^{BB}(K, \omega) \end{pmatrix}. \quad (10)$$

Once the cluster problem is solved, we calculate the coarse-grained lattice Green function as

$$\begin{aligned} \overline{G}(K, \omega) &= \begin{pmatrix} \overline{G}^{AA}(K, \omega) & \overline{G}^{AB}(K, \omega) \\ \overline{G}^{BA}(K, \omega) & \overline{G}^{BB}(K, \omega) \end{pmatrix} \\ &= \frac{N_c}{N} \sum_{\vec{k}} \left( \underline{G}_c(K, \omega)^{-1} + \underline{\Delta}(K, \omega) \right. \\ &\quad \left. - \underline{\varepsilon}_{\vec{k}} + \underline{\overline{t}}(K + \vec{k}) \right)^{-1}. \end{aligned} \quad (11)$$

It is important to note that each component of the Green function matrix above does not have the normalization of a conventional, i.e., scalar, Green function. Only the sum of the matrix components has the conventional normalization, so that  $\overline{G}(K, \omega) \sim 1/\omega$ , with the total coarse grained lattice Green function being obtained as

$$\begin{aligned} \overline{G}(K, \omega) &= \overline{G}^{AA}(K, \omega) + \overline{G}^{BB}(K, \omega) \\ &\quad + \overline{G}^{AB}(K, \omega) + \overline{G}^{BA}(K, \omega). \end{aligned} \quad (12)$$

Next, to construct the new DCA effective medium  $\underline{\Delta}(K, \omega)$ , we impose the BEB DCA ( $2 \times 2$ ) matrix self-consistency condition, requiring the disorder averaged cluster and the coarse-grained lattice Green functions to be equal

$$\underline{G}_c(K, \omega) = \overline{G}(K, \omega). \quad (13)$$

This is equivalent to a system of three coupled scalar equations

$$\overline{G}^{AA}(K, \omega) = G_c^{AA}(K, \omega), \quad (14a)$$

$$\overline{G}^{BB}(K, \omega) = G_c^{BB}(K, \omega), \quad \text{and} \quad (14b)$$

$$\overline{G}^{AB}(K, \omega) = G_c^{AB}(K, \omega). \quad (14c)$$

Note  $\overline{G}^{BA}(K, \omega) = \overline{G}^{AB}(K, \omega)$  automatically.

We then close our self-consistency loop by updating the corresponding hybridization functions for each components as

$$\begin{aligned}\Delta_n^{AA}(K, \omega) &= \Delta_o^{AA}(K, \omega) \\ &+ \xi \left( G_c^{-1}(K, \omega)^{AA} - \overline{G}^{-1}(K, \omega)^{AA} \right) \\ \Delta_n^{BB}(K, \omega) &= \Delta_o^{BB}(K, \omega) \\ &+ \xi \left( G_c^{-1}(K, \omega)^{BB} - \overline{G}^{-1}(K, \omega)^{BB} \right) \\ \Delta_n^{AB}(K, \omega) &= \Delta_o^{AB}(K, \omega) \\ &+ \xi \left( G_c^{-1}(K, \omega)^{AB} - \overline{G}^{-1}(K, \omega)^{AB} \right) \\ \Delta_n^{BA}(K, \omega) &= \Delta_n^{AB}(K, \omega)\end{aligned}\quad (15)$$

where ‘o’ and ‘n’ denote old and new respectively, and  $\xi$  is a linear mixing parameter  $0 < \xi < 1$ . We then iterate the above steps until convergence is reached.

There are two limiting cases of the above formalism which we carefully checked numerically. In the limit of  $N_c = 1$ , we should recover the original BEB result. Here the cluster Green function loses its  $K$  dependence, so that

$$\begin{pmatrix} G_c^{AA}(\omega) & 0 \\ 0 & G_c^{BB}(\omega) \end{pmatrix} = \frac{1}{N} \sum_k \left( \underline{G_c(\omega)}^{-1} + \underline{\Delta(\omega)} - \underline{\varepsilon(k)} \right)^{-1} \quad (16)$$

which is the BEB self-consistency condition. Here we used that  $\overline{\varepsilon}(K) = 0$  for  $N_c = 1$ . The second limiting case is when there is only diagonal disorder so that  $t^{AA} = t^{BB} = t^{AB} = 1$ . In this case the above formalism reduces to the original DCA scheme. We have verified numerically both these limits.

## B. Typical medium theory with off-diagonal disorder

To address the issue of electron localization, we recently developed the typical medium dynamical cluster approximation (TMDCA) and applied it to the three-dimensional Anderson model.<sup>26</sup> In Ref. 26 we have confirmed that the typical density of states vanishes for states which are localized and it is finite for extended states. In the following we generalize our TMDCA analysis to systems with off-diagonal disorder to address the question of localization and the mobility edge in such models.

First, we would like to emphasize that the crucial difference between TMDCA<sup>26</sup> and the standard DCA<sup>22</sup> procedure is the way the disorder averaged cluster Green function is calculated. In the TMDCA analysis instead of using the algebraically averaged cluster Green function in the self-consistency loop, we calculate the typical (geometrically) averaged cluster density of states

$$\rho_{typ}^c(K, \omega) = e^{\frac{1}{N_c} \sum_i \langle \ln \rho_{ii}(\omega) \rangle} \left\langle \frac{-\frac{1}{\pi} \Im G_c(K, \omega)}{\frac{1}{N_c} \sum_i \left( -\frac{1}{\pi} \Im G_{ii}(\omega) \right)} \right\rangle, \quad (17)$$

with the geometric averaging being performed over the local density of states  $\rho_{ii}^c(K, \omega) = -\frac{1}{\pi} \Im G_{ii}(\omega)$  only. Using this  $\rho_{typ}^c(K, \omega)$  the cluster averaged typical Green function is constructed via a Hilbert transform

$$G_c(K, \omega) = \int d\omega' \frac{\rho_{typ}^c(K, \omega')}{\omega - \omega'}. \quad (18)$$

In the presence of off-diagonal disorder, following BEB, the typical density of states becomes a  $2 \times 2$  matrix, which we define as

$$\underline{\rho_{typ}^c}(K, \omega) = \exp \left( \frac{1}{N_c} \sum_{i=1}^{N_c} \langle \ln \rho_{ii}(\omega) \rangle \right) \times \begin{pmatrix} \left\langle \frac{-\frac{1}{\pi} \Im G_c^{AA}(K, \omega)}{\frac{1}{N_c} \sum_{i=1}^{N_c} \left( -\frac{1}{\pi} \Im G_{ii}(\omega) \right)} \right\rangle & \left\langle \frac{-\frac{1}{\pi} \Im G_c^{AB}(K, \omega)}{\frac{1}{N_c} \sum_{i=1}^{N_c} \left( -\frac{1}{\pi} \Im G_{ii}(\omega) \right)} \right\rangle \\ \left\langle \frac{-\frac{1}{\pi} \Im G_c^{BA}(K, \omega)}{\frac{1}{N_c} \sum_{i=1}^{N_c} \left( -\frac{1}{\pi} \Im G_{ii}(\omega) \right)} \right\rangle & \left\langle \frac{-\frac{1}{\pi} \Im G_c^{BB}(K, \omega)}{\frac{1}{N_c} \sum_{i=1}^{N_c} \left( -\frac{1}{\pi} \Im G_{ii}(\omega) \right)} \right\rangle \end{pmatrix}. \quad (19)$$

Here the scalar prefactor depicts the local typical (geometrically averaged) density of states, while the matrix elements are linearly averaged over the disorder. Also notice that the cluster Green function  $(\underline{G_c})_{ij}$  and its components  $G_c^{AA}$ ,  $G_c^{BB}$  and  $G_c^{AB}$  are defined in the same way as in Eqs. (6-9).

In the next step, we construct the cluster average

Green function  $G_c(K, \omega)$  by performing Hilbert transform for each component

$$\underline{G_c}(K, \omega) = \begin{pmatrix} \int d\omega' \frac{\rho_{typ}^{AA}(K, \omega')}{\omega - \omega'} & \int d\omega' \frac{\rho_{typ}^{AB}(K, \omega')}{\omega - \omega'} \\ \int d\omega' \frac{\rho_{typ}^{BA}(K, \omega')}{\omega - \omega'} & \int d\omega' \frac{\rho_{typ}^{BB}(K, \omega')}{\omega - \omega'} \end{pmatrix} \quad (20)$$



Once the disorder averaged cluster Green function  $G_c(K, \omega)$  is obtained from Eq. 20, the self-consistency steps are the same as in the procedure for the off-diagonal disorder DCA described in the previous section: we calculate the coarse-grained lattice Green function using Eq. 11 which is then used to update the hybridization function with the effective medium via Eq. 15.

The above set of equations provide us with the generalization of the TMDCA scheme for both diagonal and off-diagonal disorder which we test numerically in the following sections. Also notice that for  $N_c = 1$  with only diagonal disorder ( $t^{AA} = t^{BB} = t^{AB} = t^{BA}$ ) the above procedure reduces to the local TMT scheme. In this case, the diagonal elements of the matrix in Eq. 19 will contribute  $c_A$  and  $c_B$ , respectively, with the off-diagonal elements being zero (at  $N_c = 1$  the off-diagonal terms vanish because at a given site the can be either  $A$  or  $B$  atom only). Hence, the typical density reduces to the local scalar prefactor only, which has exactly the same form as in the local TMT scheme.

### III. RESULTS AND DISCUSSION

To illustrate the generalized DCA and TMDCA algorithms described above, we present our results for the effects of diagonal and off-diagonal disorder in a generalized Anderson Hamiltonian (Eq. 1) for a three dimensional system with binary disorder distribution ( $V_A = -V_B$ ) and random hopping ( $t^{AA} \neq t^{BB}$ ,  $t^{AB} = t^{BA}$ ) with other parameters as specified. The results are presented and discussed in Subsections III A and III B.

#### A. DCA results for diagonal and off-diagonal disorder

The effect of off-diagonal disorder on the average density of states (DOS) calculated within the DCA ( $N_c = 32$ ) is presented in Fig. 1. The DOS we present in our results is a local density of states calculated as

$$\begin{aligned} DOS(\omega) = & -\frac{1}{\pi N_c} \sum_{K=1}^{N_c} \left( \Im \bar{G}^{AA}(K, \omega) + \Im \bar{G}^{AB}(K, \omega) \right. \\ & \left. + \Im \bar{G}^{BA}(K, \omega) + \Im \bar{G}^{BB}(K, \omega) \right). \end{aligned} \quad (21)$$

Notice that our TMDCA procedure for  $N_c = 1$  reduce to the original CPA-like BEB. For a fixed concentration  $c_A = 0.5$ , we examine the effects of off-diagonal disorder at two fixed values of the diagonal disorder potential  $V_A = 0.4$  (below the split-band limit) and  $V_A = 0.9$  (above the split-band limit). The off-diagonal randomness is modeled by changes in the hopping amplitudes  $t^{AA}, t^{BB}$  with  $t^{BA} = 0.5(t^{AA} + t^{BB})$ . For a diagonal disorder case (top panel of Fig. 1) with  $t^{AA} = t^{BB} = t^{AB} = t^{BA}$  we have two subbands contributing equally

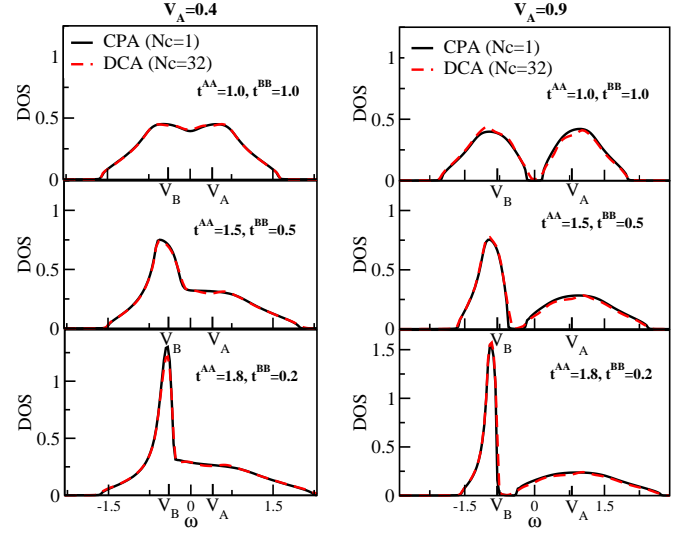


FIG. 1: (Color online). The effect of off-diagonal disorder on the average density of states calculated in the DCA scheme with  $N_c = 32$ . Our DCA results for  $N_c = 1$  corresponds to a single site CPA BEB scheme. We consider two values of local disorder potential below ( $V_A = 0.4$ ) and above ( $V_A = 0.9$ ) the band-split limit, and examine the effect of changing the off-diagonal hopping strength (which amounts to a change in the non-local potential). We start with the diagonal disorder case  $t^{AA} = t^{BB} = t^{AB} = 1.0$  and then consider two off-diagonal disorder cases:  $t^{AA} = 1.5, t^{BB} = 0.5$  and  $t^{AA} = 1.8, t^{BB} = 0.2$ , respectively. We fix  $t^{AB} = t^{BA} = 0.5(t^{AA} + t^{BB})$  and  $c_A = 0.5$ . For this parameter range of off-diagonal disorder, we do not observe a significant difference between the CPA ( $N_c = 1$ ) and the DCA ( $N_c = 32$ ) results indicating that non-local inter-site correlations are weak.

to the total DOS. While as shown in the middle and bottom panels, the change in the strength of the off-diagonal disorder leads to dramatic changes in the DOS. An increase of the AA hopping results in the broadening of the AA subband with the development of a resonance peak at the BB subband. For this parameter range both the DCA ( $N_c = 32$ ) and CPA ( $N_c = 1$ ) provide about the same results indicating that disorder-induced non-local correlations are negligible.

In Fig. 2, we show the average density of states calculated for fixed off-diagonal-disorder parameters and different diagonal disorder potentials  $V_A$ . We again compare local CPA ( $N_c = 1$ ) and the DCA ( $N_c = 32$ ) results. To benchmark our off-diagonal extension of the DCA, we compare our results with those obtained from exact diagonalization. For small  $V_A$ , there is no difference between the CPA ( $N_c = 1$ ) and the DCA ( $N_c = 32$ ) results. As local potential  $V_A$  is increased, noticeable differences start to develop. We can see that for larger  $V_A$  a gap starts to open and is more dramatic in the CPA scheme. While in the DCA ( $N_c = 32$ ) this gap is partially filled due to the incorporation of non-local inter-site correlations which are missing in the CPA. Furthermore, the DOS obtained from the DCA procedure provides finer

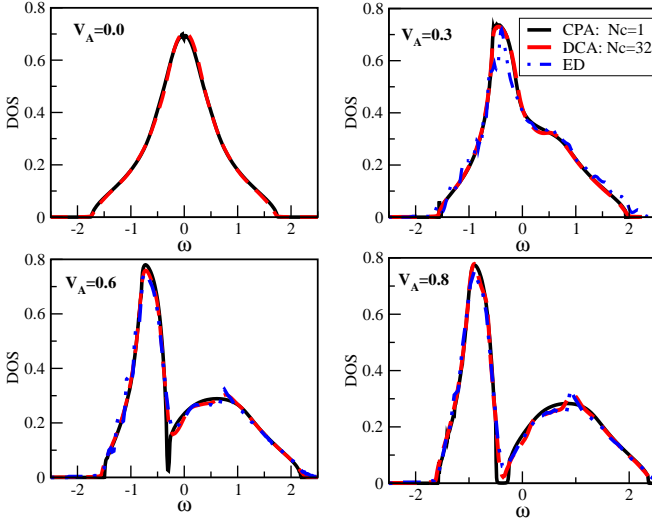


FIG. 2: (Color online). The effect of an increasing diagonal disorder potential  $V_A$  for a fixed off-diagonal disorder with  $t^{AA} = 1.5$ ,  $t^{BB} = 0.5$ ,  $t^{AB} = 0.5(t^{AA} + t^{BB})$ ,  $c_A = 0.5$ . on the the average density of states calculated with our modified DCA scheme. Results are obtained for  $N_c = 1$  (corresponding to the CPA) and  $N_c = 32$  cluster sizes. We also compare our DCA average DOS with the DOS obtained using exact diagonalization (ED) for a  $12 \times 12 \times 12$  cubic lattice cluster. For ED results, we used  $\eta = 0.01$  broadening in frequency.

structures which are in basic agreement with the DOS calculated with exact diagonalization for a cluster of size  $12 \times 12 \times 12$ . The agreement we get with ED results is a good indication of the the accuracy of our extension of the DCA to off-diagonal disorder.

### B. Typical medium finite cluster analysis of diagonal and off-diagonal disorder

To characterize the Anderson localization transition, we now explore the typical density of states (TDOS) calculated within our extension of the TMDCA presented in Sec. II B. In the typical medium analysis, the TDOS serves as the order parameter for the Anderson localization transition. In particular, the TDOS is finite for extended states and zero for states which are localized.

First we consider the behavior of the TDOS and compare it with the average DOS for diagonal disorder. In Fig. 3 we show our results for  $N_c = 1$  (left panel) and  $N_c = 32$  (right panel). Notice that  $N_c = 1$  results for TDOS correspond to the single-site TMT of Dobrosavljević *et al.*,<sup>36</sup> and for average DOS they correspond to the ordinary CPA. As expected,<sup>26,36</sup> for small disorder ( $V_A = 0.15$ ) there is not much difference between the DCA ( $N_c = 32$ ) and the TMDCA ( $N_c = 32$ ) or between the CPA and TMT for  $N_c = 1$  results. However, there are subtle differences between the results for finite  $N_c = 32$  and single site  $N_c = 1$  clusters due to incorporation of spatial correlations. As the disorder strength  $V_A$  is in-

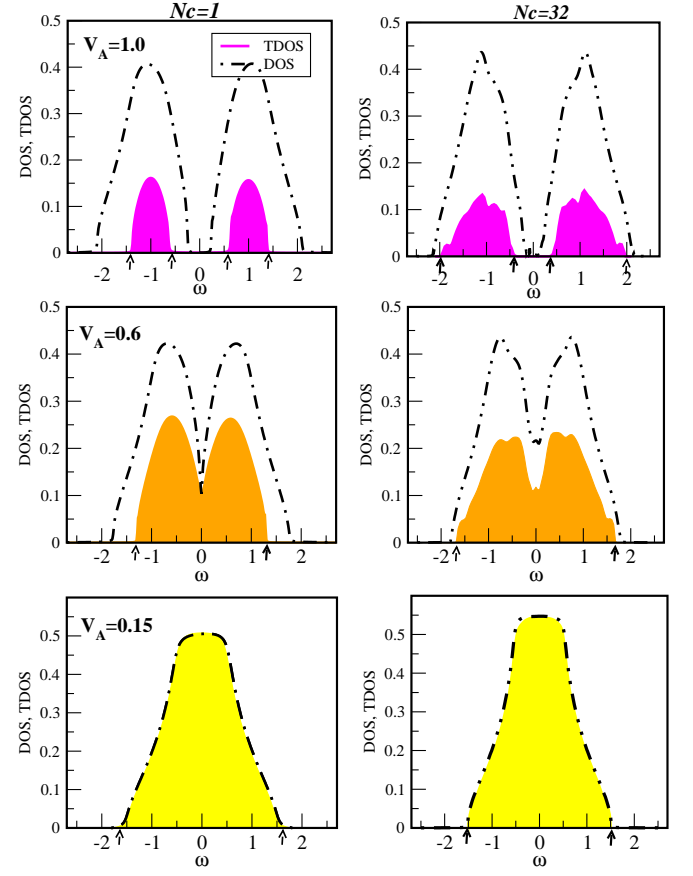


FIG. 3: (Color online). Diagonal disorder case: the average density of states (dash-dotted line) calculated within the DCA and the typical density of states (shaded regions) calculated within the TMDCA for diagonal disorder  $t^{AA} = t^{BB} = t^{AB} = t^{BA} = 1$ ,  $c_A = 0.5$  and various values of the local potential  $V_A = -V_B$  for cluster sizes  $N_c = 1$  and  $N_c = 32$ . The shaded regions represent the TDOS which is finite for the extended states and zero when the states are localized. The mobility edges extracted from the vanishing of the TDOS are marked by the arrows. The extended states region with a finite TDOS is always narrower for  $N_c = 1$  as compared to the results of a  $N_c = 32$  cluster, indicating that a single site TMT tends to overemphasize the localized states.

creased ( $V_A = 0.6$ ), the typical density of states (TDOS) becomes smaller than the average DOS and is broader for the larger cluster. Moreover, the finite cluster introduce features in the DOS which are missing in the local  $N_c = 1$  data. Regions where the TDOS is zero while the average DOS is finite indicate Anderson localized states, separated by the mobility edge (marked by arrows). For  $N_c > 1$  these localized regions are wider which indicates that the localization edge is driven to higher frequencies. This is a consequence of the tendency of non-local corrections to suppress localization. For even larger disorder  $V_A = 1$ , a gap opens in both the TDOS and the average DOS leading to the formation of four localization edges, but again the region of extended states is larger for the finite cluster, indicating that local TMT ( $N_c = 1$ ) tends

to underestimate the extended states region.

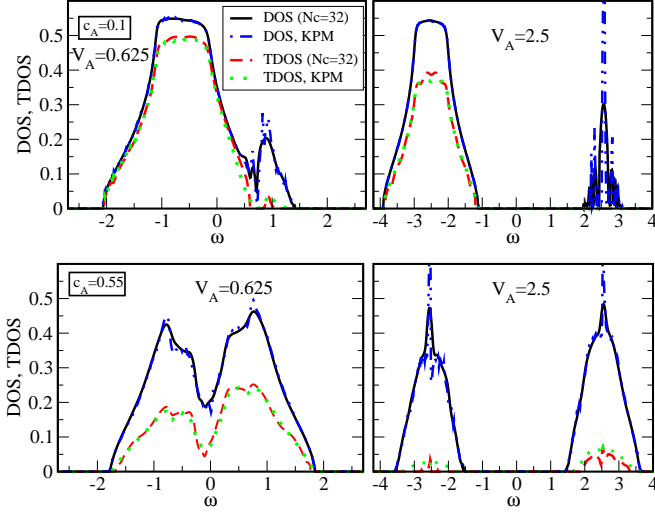


FIG. 4: (Color online). Diagonal disorder case: Comparison of the average and typical DOS calculated with the DCA/TMDCA and Kernel polynomial methods (KPM)<sup>38</sup> for diagonal disorder with  $t^{AA} = t^{BB} = t^{AB} = t^{BA} = 1$  at various values of local potential  $V_A$  and concentrations  $c_A$  for cluster size  $N_c = 32$ . The kernel polynomial method used 2048 moments on a  $48^3$  cubic lattice, and 200 independent realizations generated with 32 sites randomly sampled from each realization.

To further benchmark our results for the diagonal disorder, we show in Fig. 4 a comparison of the average and typical DOS calculated with the DCA and the TMDCA ( $N_c = 32$ ) as compared with the kernel polynomial method (KPM).<sup>38,39</sup> In the KPM analysis, instead of diagonalizing the Hamiltonian directly, the local DOS is expressed in term of an infinite series of Chebyshev polynomials. In practice, the truncated series leads to Gibbs oscillations. The KPM damps these oscillations by a modification of the expansion coefficients. Following previous studies on the Anderson model, the Jackson kernel is used.<sup>39</sup> As it is evident from the plots, our TMDCA results reproduced those from the KPM nicely showing that our formalism offers a systematic way of studying the Anderson localization transition in binary alloy systems. Such good agreement indicates a successful benchmarking of the TMDCA method.<sup>26</sup>

Next, we explore the effects of the off-diagonal disorder. In Fig. 5, we compare the typical TDOS from the TMDCA and average DOS from the DCA for several values of the diagonal disorder strength  $V_A$  at fixed off-diagonal disorder amplitudes  $t^{AA} = 1.5$ ,  $t^{BB} = 0.5$ ,  $t^{AB} = 1.0$ . To show the effect of a finite cluster with non-local correlations, we present data for single site  $N_c = 1$  and finite cluster  $N_c = 32$ . The TMT ( $N_c = 1$ ) again underestimates the extended states regime by having a narrower TDOS as compared to  $N_c = 32$ . For small disorder  $V_A$  both the DOS and the TDOS are practically the same. However, as  $V_A$  increases, significant differ-

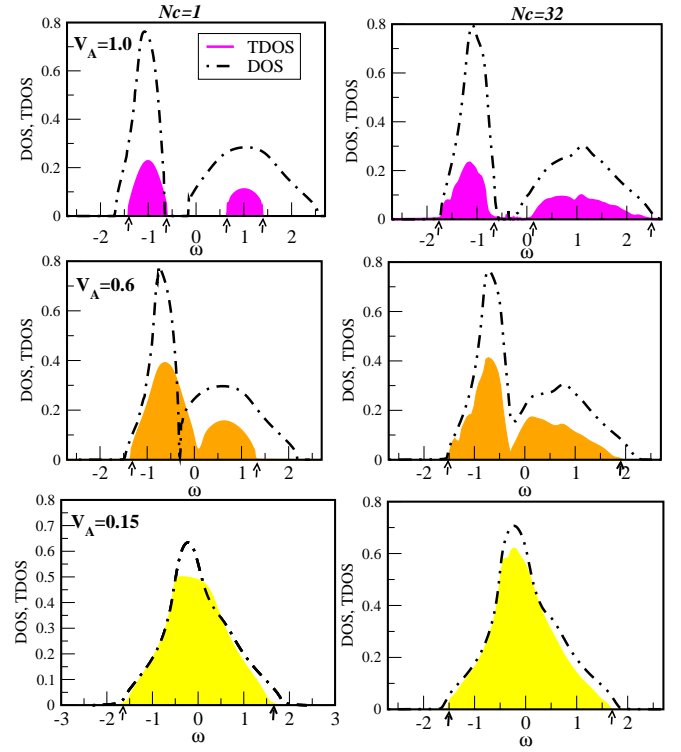


FIG. 5: (Color online). Off-diagonal disorder case: the evolution of the average density of states (dash-dotted line) and the typical density of states (shaded regions) for various values of the local potential  $V_A$  with off-diagonal disorder parameters:  $t^{AA} = 1.5$ ,  $t^{BB} = 0.5$ ,  $t^{AB} = 0.5(t^{AA} + t^{BB})$ , and  $c_A = 0.5$ . The left panel is for  $N_c = 1$  and the right panel for  $N_c = 32$ . The mobility edges are extracted as described in Fig. 3.

ences start to emerge. Increasing  $V_A$  leads to the gradual opening of the gap which is more pronounced in the  $N_c = 1$  case and for smaller disorder  $V_A = 0.6$  is partially filled for the  $N_c = 32$  cluster. As compared to the diagonal disorder case of Fig. 3, the average DOS and TDOS become asymmetric with respect to zero frequency due to the off-diagonal randomness.

In Fig. 6 we present the disorder-energy phase diagram for both diagonal (left panel) and off-diagonal (right panel) disorder calculated using the single TMT ( $N_c = 1$ ) and the non-local TMDCA ( $N_c = 72$ ). To check the accuracy of the mobility edge trajectories extracted from our typical medium analysis, we compare our data with the results obtained with the transfer matrix method (TMM).

The TMM<sup>13,40,41</sup> is a well established numerical method for calculating the correlation length and determining the mobility edge of the disorder Anderson model. Its main advantage is in its capability of capturing the effects from rather large system sizes. Thus, it provides good data for a finite size scaling analysis to capture the critical points and the corresponding exponents. In our calculations, the transmission of states down a three-dimensional bar of widths  $M = [6, 12]$  and length

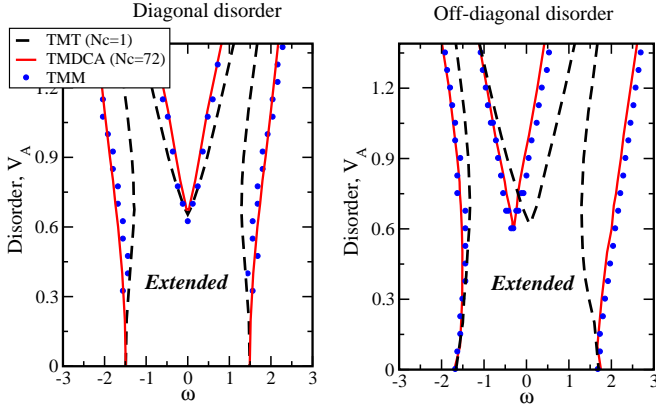


FIG. 6: (Color online). Disorder-energy phase diagram for the diagonal disorder case (left panel) and for the off-diagonal disorder case (right panel). Parameters used for the diagonal disorder case are:  $t^{AA} = t^{BB} = t^{AB} = 1.0$ , and  $c_A = 0.5$ . For the off-diagonal disorder case:  $t^{AA} = 1.5$ ,  $t^{BB} = 0.5$ ,  $t^{AB} = 1.0$ , and  $c_A = 0.5$ . We compare the mobility edges obtained from the TMT  $N_c = 1$  (dash line), TMDCA  $N_c = 72$  (solid line), and the transfer-matrix method (TMM) (dotted line). The single site  $N_c = 1$  strongly underestimates the extended states region in both the diagonal and especially in the off-diagonal disorder. The mobility edges obtained from the finite cluster TMDCA ( $N_c = 72$ ) show good agreement with those obtained from the TMM, in contrast to single site TMT. See text for parameters and details of the TMM implementation.

$L = 2 \times 10^4 M$  are studied by adding the products of the transfer matrices with random initial states. The multiplication of transfer matrices is numerically unstable. To avoid this instability, we orthogonalized the transfer matrix product every five multiplications using a Lapack QR decomposition.<sup>7</sup> The localization edge is obtained by calculating the Kramer-MacKinnon scaling parameter  $\Lambda_M$ .<sup>40</sup> This is a dimensionless quantity which should be invariant at the critical point, that is,  $\Lambda_M$  scales as a constant for  $M \rightarrow \infty$ .<sup>41</sup> Thus, we determine the boundary of the localization transition vis-à-vis the critical disorder strength<sup>42</sup> by performing a linear fit to  $\Lambda_M$  v.  $M$  data: localized states will have a negative slope and visa versa for extended states. The transfer-matrix method finite size effects are larger for weak disorder where the states decay slowly with distance and so have large values of  $\Lambda_M$  that carry a large variance in the data. Notice that the CPA and the DCA do not suffer such finite size effect limitation for small disorder and are in fact exact in this limit.

The mobility edges shown in Fig. 6 were extracted from the TDOS, with boundaries being defined by zero TDOS. As can be seen in Fig. 6, while the single-site TMT does not change much under the effect of off-diagonal disorder, the TMDCA results are significantly modified. The bands for a larger cluster become highly asymmetric with significant widening of the A subband. The local  $N_c = 1$  boundaries are narrower than those obtained for  $N_c = 72$

indicating that the TMT strongly underestimates the extended states regime in both diagonal and off-diagonal disorder. On the other hand, comparing the mobility edge boundaries for  $N_c = 72$  with those obtained using TMM, we find very good agreement. This again confirms the validity of our generalized TMDCA.

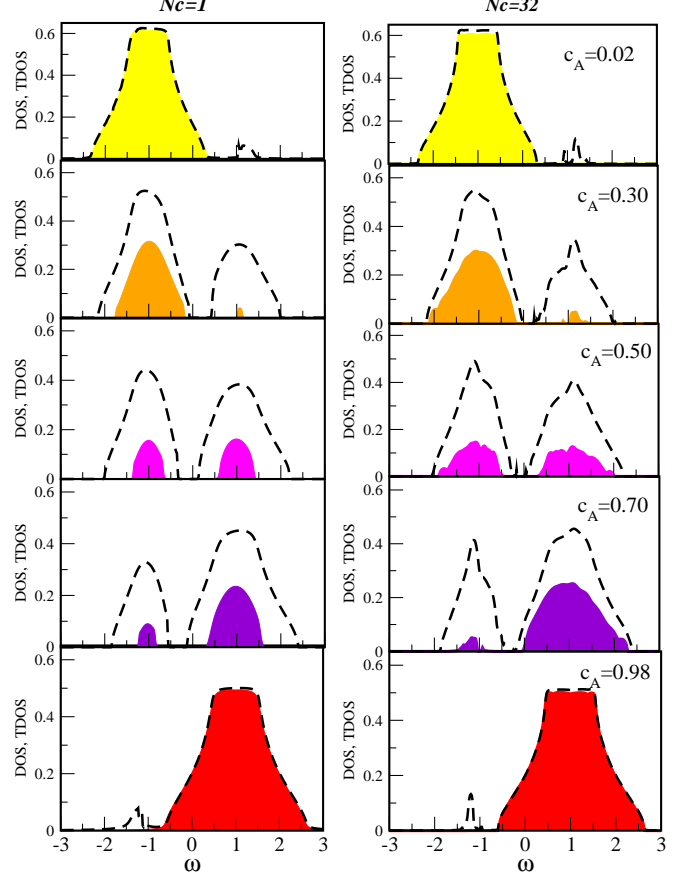


FIG. 7: (Color online). The average DOS (dot-dashed lines) and the typical DOS (shaded regions) for various values of the concentration  $c_A$  with off-diagonal disorder parameters  $t^{AA} = 1.1$ ,  $t^{BB} = 0.9$  and  $t^{AB} = 1.0$ , at fixed local potential  $V_A = 1.0$  for  $N_c = 1$  (left panel) and  $N_c = 32$  (right panel).

Next, we consider the effect of off-diagonal disorder at various concentrations  $c_A$ . In Fig. 7, we show the typical and average DOS for several values of  $c_A$  calculated with the TMDCA and the DCA, respectively. As expected, when  $c_A \rightarrow 0$ , we obtain a pure  $B$  subband contribution (the top panel). Upon gradual increase of the  $c_A$  concentration, the number of states in the  $A$  sub-band grows until  $B$ -subband becomes a minority for  $c_A > 0.5$  and completely disappears at  $c_A \rightarrow 1$  (the bottom panel). Again, we see that a finite cluster  $N_c = 32$  provides a more accurate description (with finite details in DOS and broader regions of extended states in TDOS) in both average DOS and TDOS. The associated contour plots for the evolution of the TDOS in the concentrations range  $0 \leq c_A \leq 1$  are shown in Fig. 8. The essence of these plots is to show the overall evolution of the typical and



average DOS for a fixed local potential and off-diagonal disorder parameters as a function of the concentration  $c_A$ . In the limit of  $c_A \rightarrow 0$ , only the B-subband centered around  $\omega = -V_A$  survives, and for  $c_A \rightarrow 1$ , only the A-subband centered around  $\omega = V_A$  is present. For intermediate concentrations, we clearly have contributions to the total typical density of states from both species, as expected.

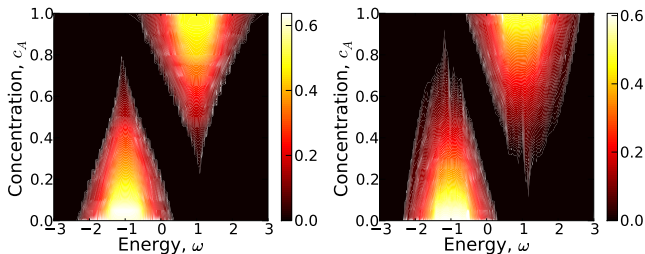


FIG. 8: (Color online). The evolution of the typical density of states for  $N_c = 1$  (left panel) and  $N_c = 32$  (right panel) with the change in the concentration  $0 < c_A < 1$  at fixed diagonal and off-diagonal disorder parameters:  $t^{AA} = 1.1$ ,  $t^{BB} = 0.9$ ,  $t^{AB} = 1.0$  and  $V_A = 1.0$

Finally, we would like to comment on the possible further development of the presented scheme. After certain generalizations our current implementation of the typical medium dynamical cluster approximation for off-diagonal disorder can serve as the natural formalism for multiband (multiorbital) systems.<sup>43</sup> Such an extension is crucial for studying disorder and localization effects in real materials. Further development towards this direction will be the subject of future publications.

#### IV. CONCLUSION

A proper theoretical description of disordered materials requires the inclusion of both diagonal and off-diagonal randomness. In this paper, we have extended the BEB single site CPA scheme to a finite cluster DCA that incorporates the effect of non-local disorder. Applying the generalized DCA scheme to a single band tight binding Hamiltonian with configuration-dependent hopping amplitudes, we have considered the effects of non-local disorder and the interplay of diagonal and off-diagonal disorder on the average density of states. By

comparing our numerical results with those from exact diagonalization, we have established the accuracy of our method.

To study the effect of disorder on electron localization and to determine the mobility edge in systems with both diagonal and off-diagonal randomness, we have also extended our recently developed TMDCA to included off-diagonal randomness. Within the TMDCA the typical DOS vanishes for localized states, and is finite for states which are extended. Employing the typical DOS as an order parameter for Anderson localization, we have constructed the disorder-energy phase diagram for systems with both diagonal and off-diagonal disorder. We have also demonstrated the inability of the single site CPA and the TMT methods to capture accurately the localization and disorder effects in both the average and the typical DOS, respectively. Comparing our results with kernel polynomial, exact diagonalization, and transfer-matrix methods we find a remarkably good agreement with our extended DCA and TMDCA. To the best of our knowledge, this is the first numerically accurate investigation of the Anderson localization in systems with off-diagonal disorder within the framework of the typical medium analysis. We believe that the extended TMDCA scheme presents a powerful tool for treating both diagonal and off-diagonal disorder on equal footing, and can be easily extended to study localization in multi-band systems.

#### Acknowledgments

We thank A. Gonis for useful discussion and directing us to the BEB formalism, we also thank Shuxiang Yang, Wei Ku, and Tom Berlijn for useful discussions. This work is supported by DOE SciDAC grant DE-FC02-10ER25916 (MJ) and BES CMCSN grant DE-AC02-98CH10886 (HT). Additional support was provided by NSF EPSCoR Cooperative Agreement No. EPS-1003897 (HT, CE, CM), and NSF OISE-0952300 (JM). This work used the Extreme Science and Engineering Discovery Environment (XSEDE), which is supported by National Science Foundation grant number ACI-1053575, the high performance computational resources provided by the Louisiana Optical Network Initiative (<http://www.loni.org>), and HPC@LSU computing.

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